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Title: (U) Differences in the Use of Isotopic Vectors Demonstrated with an Analytic k Problem (And Verification of SENSMG and MCNP6's KSEN)

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SUBJECT: (U) Differences in the Use of Isotopic χ Vectors Demonstrated with an Analytic k_∞ Problem (And Verification of SENSMG and MCNP6's KSEN)

I. Introduction

Comparisons of responses and first-order sensitivities of responses to the neutron fission spectrum (χ) have been done using different transport methods. Kodeli and Slavič compared sensitivities from Monte Carlo, deterministic, and method of characteristics of k_{eff} in the SNEAK-7 benchmark, and the agreement was reasonable.[1] Yamamoto compared deterministic and Monte Carlo sensitivities of k- and α-eigenvalues to the fission χ, but only for material (i.e. single-isotope) values of the fission χ.[2,3] Haeck et al. compared Monte Carlo and deterministic sensitivities of k_{eff} to the fission χ of individual isotopes for several benchmarks, and the agreement was excellent (except, strangely, for U-236).[4,5] Kiedrowski and Brown compared Monte Carlo and analytic sensitivities of k_∞ to the fission χ in analytic problems, but only for material values of the fission χ.[6,7]

There is a difference in how Monte Carlo and deterministic codes use the fission χ that yields different results, even using the same nuclear data. The difference manifests itself when a fission χ vector is used rather than a matrix and when a material comprises multiple isotopes. References 1 through 7 did not observe this effect because they were able to use fission χ matrices rather than vectors[4,5]; they only looked at one-isotope problems[2,3,6,7]; or the codes were not using the same nuclear data.[1]

This report discusses the difference and presents an analytic multigroup two-isotope neutron k_∞ problem that demonstrates it. The sensitivity of k_∞ to the isotopic fission χ is obtained analytically for a fission χ vector and numerically (using a central difference) for a fission χ matrix. The sensitivities are compared with results of the multigroup neutron sensitivity code[8,9] SENSMG (using the multigroup

discrete-ordinates PARTISN code[10]) and the KSEN capability[11] of the MCNP6.2 Monte Carlo code[12] (in multigroup mode).

Section II derives k_∞ using a fission χ vector, and Sec. III derives k_∞ using a fission χ matrix, both for an arbitrary number of energy groups. Section IV discusses how MCNP and PARTISN differ in their use of χ vectors. Section V presents results of an eight-group test problem. Section VI is a summary and conclusions. The input files for the test problem are listed in Appendix A. Appendix B presents SENSMG results for a three-group test problem used previously[6] for verification of KSEN.

II. k_∞ Using χ Vector

The multigroup transport equation for k_∞ for a homogeneous material with isotropic scattering and a fission χ vector for an arbitrary number of energy groups is

$$\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)\bar{\phi} = \frac{1}{k_\infty}\bar{\chi}\,\overline{\nu\Sigma_f}^T\bar{\phi}, \tag{1}$$

where $\overline{\nu\Sigma_f}$ is the vector of material $\nu\Sigma_f^g$ cross sections; $\overline{\overline{\Sigma}}_t$ is the diagonal matrix of material Σ_t^g cross sections; $\overline{\overline{\Sigma}}_s$ is the matrix of material group-to-group scattering cross sections; $\bar{\chi}$ is the vector of material fission χ^g elements; and superscript *T* indicates transpose. The solution of Eq. (1) for k_∞ is[13]

$$k_\infty = \overline{\nu\Sigma_f}^T\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)^{-1}\bar{\chi}. \tag{2}$$

The material fission $\bar{\chi}$ vector is composed of elements χ^g computed from the isotopic fission vectors $\overline{\chi_i}$ with elements χ_i^g using

$$\chi^g = \frac{\sum_{i=1}^{I}\chi_i^g N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}, \tag{3}$$

where $f_i^{g'}$ is the spectrum weighting function and *I* is the number of fissionable isotopes in the material. The spectrum weighting function is only available through the Nuclear Data Interface (NDI) at LANL. For other cross section libraries, the spectrum weighting function is set to 1.

The product $\bar{\chi}\,\overline{\nu\Sigma_f}^T$ is called the *fission transfer matrix*. When isotopic fission χ vectors are used to create a material fission χ vector, the fission transfer matrix is

$$\overline{\chi}\,\overline{\nu\Sigma_f}^T = \begin{bmatrix} \chi^1 \\ \chi^2 \\ \vdots \\ \chi^G \end{bmatrix} \begin{bmatrix} \nu\Sigma_f^1 & \nu\Sigma_f^2 & \cdots & \nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \chi^1\nu\Sigma_f^1 & \chi^1\nu\Sigma_f^2 & \cdots & \chi^1\nu\Sigma_f^G \\ \chi^2\nu\Sigma_f^1 & \chi^2\nu\Sigma_f^2 & \cdots & \chi^2\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \chi^G\nu\Sigma_f^1 & \chi^G\nu\Sigma_f^2 & \cdots & \chi^G\nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \dfrac{\sum_{i=1}^{I}\chi_i^1 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^1 & \dfrac{\sum_{i=1}^{I}\chi_i^1 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^2 & \cdots & \dfrac{\sum_{i=1}^{I}\chi_i^1 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^G \\ \dfrac{\sum_{i=1}^{I}\chi_i^2 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^1 & \dfrac{\sum_{i=1}^{I}\chi_i^2 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^2 & \cdots & \dfrac{\sum_{i=1}^{I}\chi_i^2 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\sum_{i=1}^{I}\chi_i^G N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^1 & \dfrac{\sum_{i=1}^{I}\chi_i^G N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^2 & \cdots & \dfrac{\sum_{i=1}^{I}\chi_i^G N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}\nu\Sigma_f^G \end{bmatrix}. \quad (4)$$

If there is only one fissionable isotope in the material, Eq. (3) reduces to $\chi^g = \chi_1^g$, as expected. If there is only one energy group, regardless of the number of isotopes, then $\chi^1 = \chi_i^1 = 1$, which is not an interesting case.

The vector of partial derivatives of k_∞ with respect to each element of $\overline{\chi}$ is, from Eq. (2),

$$\overline{\partial k_\infty/\partial\chi} = \overline{\nu\Sigma_f}^T \left(\overline{\overline{\Sigma}_t} - \overline{\overline{\Sigma}_s}\right)^{-1}. \quad (5)$$

The derivative of χ^g with respect to χ_i^g for a particular isotope is, from Eq. (3),

$$\frac{\partial\chi^g}{\partial\chi_i^g} = \frac{N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}{\sum_{i=1}^{I}N_i\sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'}f_i^{g'}}. \quad (6)$$

Using the chain rule, the derivative of k_∞ with respect to χ_i^g is

$$\frac{\partial k_\infty}{\partial\chi_i^g} = \frac{\partial k_\infty}{\partial\chi^g}\frac{\partial\chi^g}{\partial\chi_i^g}, \quad (7)$$

where $\partial k_\infty/\partial\chi^g$ indicates each element of the vector $\overline{\partial k_\infty/\partial\chi}$ of Eq. (5).

Equations (5) and (7) are unconstrained derivatives[14] that do not account for the fact that $\overline{\chi}$ and $\overline{\chi_i}$ are normalized spectra.

Using Eq. (7), the unconstrained relative sensitivity of k_∞ to a change in χ_i^g is

$$S_{k_\infty,\chi_i^g} \equiv \frac{\chi_i^g}{k_\infty}\frac{\partial k_\infty}{\partial \chi_i^g} = \frac{\chi_i^g}{k_\infty}\frac{\partial k_\infty}{\partial \chi^g}\frac{\partial \chi^g}{\partial \chi_i^g}. \tag{8}$$

The *constrained* relative sensitivity of k_∞ to a change in χ_i^g is

$$S^{FN}_{k_\infty,\chi_i^g} = S_{k_\infty,\chi_i^g} - \chi_i^g \sum_{g=1}^{G} S_{k_\infty,\chi_i^g}, \tag{9}$$

where *FN* indicates full normalization.[14] This sensitivity accounts for the fact that changing χ_i^g causes the other elements of $\overline{\chi_i}$ to be changed as well, to preserve the normalization.

III. k_∞ Using χ Matrix

When the full matrix fission $\overline{\overline{\chi}}$ is used, there is not a closed-form solution for k_∞. The multigroup transport equation for k_∞ becomes

$$\left(\overline{\overline{\Sigma_t}} - \overline{\overline{\Sigma_s}}\right)\overline{\phi} = \frac{1}{k_\infty}\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma_f}}\,\overline{\phi}, \tag{10}$$

where $\overline{\overline{\nu\Sigma_f}}$ is the diagonal matrix of material $\nu\Sigma_f^g$ cross sections. Equation (10) is solved iteratively, starting with initial guesses for $\overline{\phi}$ and k_∞:

$$\overline{\phi}^{k+1} = \frac{1}{k_\infty^k}\left(\overline{\overline{\Sigma_t}} - \overline{\overline{\Sigma_s}}\right)^{-1}\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma_f}}\,\overline{\phi}^k, \tag{11}$$

where superscript *k* is the iteration index. At each iteration, the updated k_∞^{k+1} is computed using

$$k_\infty = \left[\overline{I}^T\left(\overline{\overline{\Sigma_t}} - \overline{\overline{\Sigma_s}}\right)\overline{\phi}\right]^{-1}\left[\overline{I}^T\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma_f}}\,\overline{\phi}\right], \tag{12}$$

where $\overline{I}$ is a vector whose elements are all unity.

There is no convenient expression for $\partial k_\infty / \partial \chi^{g'\to g}$.

The material $\chi^{g'\to g}$ is computed from the isotopic $\chi_i^{g'\to g}$ values using

$$\chi^{g'\to g} = \frac{\sum_{i=1}^{I}\chi_i^{g'\to g}N_i\nu\sigma_{f,i}^{g'}}{\sum_{i=1}^{I}N_i\nu\sigma_{f,i}^{g'}} = \frac{\sum_{i=1}^{I}\chi_i^{g'\to g}N_i\nu\sigma_{f,i}^{g'}}{\nu\Sigma_f^{g'}}. \tag{13}$$

Note that Eq. (13) does not have the spectrum weighting function $f_i^{g'}$ that appears in Eq. (3). When isotopic fission χ matrices are used to create a material fission χ matrix, the fission transfer matrix is [using Eq. (13)]

$$\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma_f}} = \begin{bmatrix} \chi^{1\to1} & \chi^{2\to1} & \cdots & \chi^{G\to1} \\ \chi^{1\to2} & \chi^{2\to2} & \cdots & \chi^{G\to2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi^{1\to G} & \chi^{2\to G} & \cdots & \chi^{G\to G} \end{bmatrix} \begin{bmatrix} \nu\Sigma_f^1 & 0 & \cdots & 0 \\ 0 & \nu\Sigma_f^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \chi^{1\to1}\nu\Sigma_f^1 & \chi^{2\to1}\nu\Sigma_f^2 & \cdots & \chi^{G\to1}\nu\Sigma_f^G \\ \chi^{1\to2}\nu\Sigma_f^1 & \chi^{2\to2}\nu\Sigma_f^2 & \cdots & \chi^{G\to2}\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \chi^{1\to G}\nu\Sigma_f^1 & \chi^{2\to G}\nu\Sigma_f^2 & \cdots & \chi^{G\to G}\nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{i=1}^{I} \chi_i^{1\to1} N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^{2\to1} N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^{G\to1} N_i \nu\sigma_{f,i}^G \\ \sum_{i=1}^{I} \chi_i^{1\to2} N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^{2\to2} N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^{G\to2} N_i \nu\sigma_{f,i}^G \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{I} \chi_i^{1\to G} N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^{2\to G} N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^{G\to G} N_i \nu\sigma_{f,i}^G \end{bmatrix}. \tag{14}$$

If there is only one fissionable isotope in the material, Eq. (13) reduces to $\chi^{g'\to g} = \chi_1^{g'\to g}$, as expected. If there is only one energy group, regardless of the number of isotopes, then $\chi^{1\to1} = \chi_i^{1\to1} = 1$, again not an interesting case.

The elements of each isotopic fission χ matrix $\overline{\overline{\chi_i}}$ are

$$\overline{\overline{\chi_i}} = \begin{bmatrix} \chi_i^{1\to1} & \chi_i^{2\to1} & \cdots & \chi_i^{G\to1} \\ \chi_i^{1\to2} & \chi_i^{2\to2} & \cdots & \chi_i^{G\to2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_i^{1\to G} & \chi_i^{2\to G} & \cdots & \chi_i^{G\to G} \end{bmatrix}. \tag{15}$$

However, if only the vector $\overline{\chi_i}$ is available for each isotope, then every group g' has the same contribution to group g. The elements of $\overline{\overline{\chi_i}}$ become

$$\overline{\overline{\chi_i}} = \begin{bmatrix} \chi_i^{1\to1} & \chi_i^{1\to1} & \cdots & \chi_i^{1\to1} \\ \chi_i^{2\to2} & \chi_i^{2\to2} & \cdots & \chi_i^{2\to2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_i^{G\to G} & \chi_i^{G\to G} & \cdots & \chi_i^{G\to G} \end{bmatrix} = \begin{bmatrix} \chi_i^1 & \chi_i^1 & \cdots & \chi_i^1 \\ \chi_i^2 & \chi_i^2 & \cdots & \chi_i^2 \\ \vdots & \vdots & \ddots & \vdots \\ \chi_i^G & \chi_i^G & \cdots & \chi_i^G \end{bmatrix}. \tag{16}$$

Using Eq. (13), the material χ matrix is

$$\overline{\overline{\chi}} = \begin{bmatrix} \dfrac{\sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \dfrac{\sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \dfrac{\sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \\ \dfrac{\sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \dfrac{\sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \dfrac{\sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \dfrac{\sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \dfrac{\sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \end{bmatrix}, \tag{17}$$

and the fission transfer matrix is

$$\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma_f}} = \begin{bmatrix} \sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^G \\ \sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^G \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^G \end{bmatrix}. \tag{18}$$

In general, the columns of $\overline{\overline{\chi}}$ [Eq. (17)] are not the same, unlike the columns of $\overline{\overline{\chi_i}}$ [Eq. (16)]. Thus, even though only χ vectors for isotopes may be given, a material χ matrix may result, depending on assumptions or conventions. In particular, it will be shown in Sec. IV that multigroup MCNP converts input isotopic χ vectors to a material χ matrix, while multigroup PARTISN converts input isotopic χ vectors to a material χ vector.

If there is only one fissionable isotope in the material, Eq. (17) reduces to $\overline{\overline{\chi}} = \overline{\overline{\chi_1}}$. Then Eq. (18) is equal to Eq. (4), and therefore Eq. (10) has the same solution and sensitivities as Eq. (1). This equality also holds if there is only one energy group, regardless of the number of isotopes.

Because there is no analytic expression for $\partial k_\infty / \partial \chi^{g' \to g}$, the sensitivity of k_∞ to each χ_i^g for the test problem in Sec. V was determined using a central difference. Full normalization was used. The procedure is detailed in Ref. 14. First, perturb χ_i^g to $\chi_i^g + \Delta\chi_i^g$; then, normalize every element of the perturbed $\overline{\chi_i}$. Solve Eqs. (11) and (12) with the perturbed, renormalized $\overline{\chi_i}$ to compute $k_{\infty,+}$. Do the same with the opposite perturbation $-\Delta\chi_i^g$ to compute $k_{\infty,-}$. The relative sensitivity is approximately

$$S_{k_\infty,\chi_i^g}^{FN} \approx \frac{\chi_i^g}{k_\infty} \frac{k_{\infty,+} - k_{\infty,-}}{2\Delta\chi_i^g}. \tag{19}$$

The accuracy of Eq. (19) depends on the linearity of the three points $(-\Delta\chi_i^g, k_{\infty,-})$, $(0, k_\infty)$, and $(\Delta\chi_i^g, k_{\infty,+})$. Note that Eq. (19) uses the input $\Delta\chi_i^g$ in the denominator, not the change in χ_i^g after the renormalization.

IV. How MCNP and PARTISN Differ in Their Use of Isotopic χ Vectors

In multigroup or continuous-energy mode, MCNP first samples the neutron's distance to collision in the material, then samples what type of collision occurred. If it is fission, then it samples for the fissioning isotope at incoming neutron energy g using probabilities $N_i\nu\sigma_{f,i}^g \Big/ \nu\Sigma_f^g$, $i = 1,\ldots,I$. Then it samples for the outgoing energy group g' from that isotope's χ vector (in multigroup). Given a fission event and incoming group g, then, the probability of choosing isotope i and outgoing group g' is $\chi_i^{g'} N_i\nu\sigma_{f,i}^g \Big/ \nu\Sigma_f^g$. The overall probability of choosing outgoing group g' is the sum over all fissionable isotopes: $\sum_{i=1}^{I} \chi_i^{g'} N_i\nu\sigma_{f,i}^g \Big/ \nu\Sigma_f^g$. Thus, in multigroup MCNP, even when isotopic χ vectors are given, the fission χ is effectively the matrix Eq. (17) and the fission transfer matrix is effectively Eq. (18).

The versions of PARTISN available at LANL use keyword `fissdata` in block 3 to specify how the fission χ should be treated. When `fissdata` = 0, PARTISN reads the fission transfer matrix for each isotope directly from the NDI and creates a material fission transfer matrix. When `fissdata` = 1, PARTISN reads the fission χ matrix and $\nu\sigma_f$ entries for each isotope from the NDI and constructs a material χ matrix and $\nu\Sigma_f$ entries. The result of both of these options is that the fission transfer matrix is given by Eq. (14). When `fissdata` = 2, PARTISN reads the fission χ vector, $\nu\sigma_f$ entries, and the spectrum weighting function for each isotope from the NDI and constructs material χ vector elements, using Eq. (3), and $\nu\Sigma_f$ entries. The result of this option is that the fission transfer matrix is given by Eq. (4).

The version of PARTISN available to external users is 5.97, which uses `nochimat` in block 3 to specify whether to use a χ matrix. However, the NDI is still needed to input a χ matrix. Thus, external users, and internal users who are not using the NDI, produce material χ vectors without the spectrum weighting function $f_i^{g'}$.

Even when the spectrum weighting function $f_i^{g'}$ is unity, Eq. (4) differs significantly from Eq. (18).

There is presently no means in PARTISN to use Eq. (18) as the fission transfer matrix. We propose a new option for the use of fission data that would be chosen with `fissdata` = 3. It would cause PARTISN to read isotopic χ vectors from either the NDI or a user-supplied cross section library (in any currently accepted format) and construct the fission transfer matrix using Eq. (18) instead of Eq. (4). The advantage of this option is that it would allow PARTISN to replicate MCNP results.

V. Eight-Group, Two-Isotope Test Problem

This test problem was a slab with width 1 cm with reflecting boundary conditions. The material was plutonium with the composition given in Table I. Its mass density was 14 g/cm^3. The full SENSMG input file is listed in the appendix. Reflective boundary conditions are not a standard feature of SENSMG; the SENSMG source code was modified to compute k_∞. An angular quadrature of S_{256} and fine mesh spacing of 0.0005 cm were used (the source code was modified to set that mesh spacing). A convergence criterion of 10^{-10} was used.

Table I. Isotope Densities.

Isotope	Density (atoms/b·cm)
Pu-239	0.03385770516
Pu-240	0.001404851530

MENDF71X cross sections collapsed to eight groups were used. A PARTISN input file for the base case that gives the relevant eight-group material cross sections is listed in the appendix. The `simple_ace_mg.pl` script[15] was used to generate isotopic multigroup ACE-formatted cross section libraries for MCNP. A script that calls the `simple_ace_mg.pl` script with eight-group isotopic cross sections is listed in the appendix. These scripts input isotopic fission χ vectors, not matrices.

The isotopic cross sections are listed in the PARTISN input and the `simple_ace_mg.pl` script inputs in Appendix A. The former gives the material fission χ vector. The spectrum weighting functions are listed separately in Appendix A.

Analytic k_∞ values for the two cases are compared in Table II. The difference is computed relative to the average:

$$\text{Difference} = \frac{\left(R_1 - R_2\right)}{\frac{1}{2}\left(R_1 + R_2\right)}, \tag{20}$$

where R_1 and R_2 are any two values to be compared. There is a very small difference between the two uses of the isotopic fission χ vectors. The difference is real, not just round-off (but round-off does contribute to some of the difference). Some, but not all, of the difference is because of the use of the spectrum weighting function $f_i^{g'}$ in Eq. (3).

Table II. Analytic k_∞ Values.

Equation	Value	Equation	Value
Vector [Eq. (2)], with f	2.94459933	Vector [Eq. (2)], $f = 1$	2.94460099
Matrix [Eq. (12)]	2.94460193	Matrix [Eq. (12)]	2.94460193
Difference	–0.00008814%	Difference	–0.00003192%

The problem was run using isotopic fission χ vectors in PARTISN using the SENSMG input file and command line listed in Appendix A (most importantly for this report, `-fissdata 2` and `-ngroup 8`). In this run, PARTISN constructed the material data from the isotopic nuclear data found in the NDI. The result is compared with the analytic result from Sec. II in Table III. The only difference is due to the finite number of digits in the PARTISN output.

Table III. k_∞, Deterministic Transport.

Calculation	Value	Difference
Analytic[(a)]	2.9445993	N/A
PARTISN	2.9445993	–0.000001%

(a) From Eq. (2), using the actual spectrum weighting function in Eq. (3).

The problem was run using the isotopic χ vectors in MCNP. The result is compared with the analytic result from Sec. III in Table IV. The MCNP result is the average of 11 calculations, each having a relative uncertainty of ±0.00001. The MCNP result is within one standard deviation of the analytic value. But it is also very close to the vector analytic value, the difference being 0.000362% and 1.07σ.

Table IV. k_∞, Monte Carlo Transport.

Calculation	Value	Difference	Difference ($N\sigma$)
Analytic[(a)]	2.94460	N/A	N/A
MCNP	2.94461 ± 0.00001	0.000274%	0.81

(a) From Eq. (12).

In summary, there is a very small difference in k_∞ when isotopic χ vectors are used in Eq. (3) versus Eq. (17) to compute the material χ. The difference is too small to be seen with the MCNP calculation. There is also a small difference introduced by the spectrum weighting function.

The difference in sensitivities is larger. The sensitivities for the vector χ were computed using Eq (9) (with other equations in Sec. II). The sensitivities for the matrix χ were computed using Eq. (19) (with other equations in Sec. III). They are compared in Table V for the case when the NDI spectrum weighting function is used. The difference uses Eq. (20). The vector χ sensitivities are 2% greater than the matrix χ sensitivities for Pu-239, but the matrix χ sensitivities are a factor of 3.7 greater than the vector χ sensitivities for Pu-240.

The vector calculation was repeated without the spectrum weighting function and those results are compared in Table VI. They are closer, but the sensitivities for the Pu-240 fission spectrum when vector χ is used are still 26% smaller than when matrix χ is used.

Much of the difference in the sensitivities is due to the spectrum weighting function $f_i^{g'}$ in Eq. (3). However, there is still a significant difference when $f = 1$. The deterministic and Monte Carlo codes are solving different equations.

Table V. Constrained Sensitivities of k_∞ to χ, Analytic, Using the NDI Spectrum Weighting Function (Full Normalization) (%/%).

Isotope	Group	Vector χ, with f	Matrix χ	Difference
Pu-239	1	1.035708E-04	1.017157E-04	1.8074%
	2	1.045315E-03	1.026591E-03	1.8074%
	3	2.685757E-02	2.637802E-02	1.8016%
	4	–1.132364E-02	–1.112195E-02	1.7971%
	5	–1.043250E-02	–1.024650E-02	1.7990%
	6	–5.630149E-03	–5.529357E-03	1.8064%
	7	–5.853621E-04	–5.748772E-04	1.8074%
	8	–3.480244E-05	–3.417906E-05	1.8074%
Pu-240	1	7.442050E-07	2.762766E-06	–115.1%
	2	7.222675E-06	2.681326E-05	–115.1%
	3	1.772846E-04	6.581838E-04	–115.1%
	4	–7.489392E-05	–2.780627E-04	–115.1%
	5	–6.907309E-05	–2.564481E-04	–115.1%
	6	–3.718477E-05	–1.380452E-04	–115.1%
	7	–3.868789E-06	–1.436239E-05	–115.1%
	8	–2.309438E-07	–8.573494E-07	–115.1%

Table VI. Constrained Sensitivities of k_∞ to χ, Analytic, Not Using the NDI Spectrum Weighting Function (Full Normalization) (%/%).

Isotope	Group	Vector χ, $f = 1$	Matrix χ	Difference
Pu-239	1	1.023819E-04	1.017157E-04	0.65285%
	2	1.033315E-03	1.026591E-03	0.65284%
	3	2.654926E-02	2.637802E-02	0.64707%
	4	–1.119365E-02	–1.112195E-02	0.64257%
	5	–1.031274E-02	–1.024650E-02	0.64446%
	6	–5.565518E-03	–5.529357E-03	0.65186%
	7	–5.786425E-04	–5.748772E-04	0.65283%
	8	–3.440293E-05	–3.417906E-05	0.65285%
Pu-240	1	2.037760E-06	2.762766E-06	–30.205%
	2	1.977692E-05	2.681326E-05	–30.205%
	3	4.854356E-04	6.581838E-04	–30.211%
	4	–2.050723E-04	–2.780627E-04	–30.215%
	5	–1.891339E-04	–2.564481E-04	–30.214%
	6	–1.018182E-04	–1.380452E-04	–30.206%
	7	–1.059340E-05	–1.436239E-05	–30.205%
	8	–6.323635E-07	–8.573494E-07	–30.205%

The analytic results are now used for code verification. Constrained sensitivities of k_∞ to elements of the isotopic χ fission vectors computed using SENSMG are compared with the analytic values in Table VII (the spectrum weight function was included). The agreement is excellent. Constrained sensitivities of k_∞ to elements of the isotopic χ fission vectors computed using the KSEN capability of MCNP6.2 are compared with central differences of the analytic values in Table VIII. The agreement is excellent. Differences on Tables VI and VII are relative to the analytic values.

Table VII. Constrained Sensitivities of k_∞ to χ, Deterministic Transport (Full Normalization) (%/%).

Isotope	Group	Analytic	SENSMG	Difference
Pu-239	1	1.035708E-04	1.035708E-04	–0.000035%
	2	1.045315E-03	1.045315E-03	0.000003%
	3	2.685757E-02	2.685757E-02	0.000011%
	4	–1.132364E-02	–1.132364E-02	0.000034%
	5	–1.043250E-02	–1.043250E-02	–0.000026%
	6	–5.630149E-03	–5.630149E-03	–0.000005%
	7	–5.853621E-04	–5.853621E-04	–0.000006%
	8	–3.480244E-05	–3.480244E-05	–0.000008%
Pu-240	1	7.442050E-07	7.442050E-07	0.000001%
	2	7.222675E-06	7.222675E-06	–0.000001%
	3	1.772846E-04	1.772846E-04	–0.000021%
	4	–7.489392E-05	–7.489392E-05	0.000000%
	5	–6.907309E-05	–6.907309E-05	–0.000005%
	6	–3.718477E-05	–3.718477E-05	–0.000002%
	7	–3.868789E-06	–3.868789E-06	0.000000%
	8	–2.309438E-07	–2.309438E-07	–0.000008%

Table VIII. Constrained Sensitivities of k_∞ to χ, Monte Carlo Transport (Full Normalization) (%/%).

Isotope	Group	Analytic CD	KSEN	Difference	Difference ($N\sigma$)
Pu-239	1	1.01716E-04	1.0212E-04 ± 1.04%	0.3975%	0.38
	2	1.02659E-03	1.0256E-03 ± 0.33%	–0.0966%	–0.29
	3	2.63780E-02	2.6405E-02 ± 0.12%	0.1023%	0.85
	4	–1.11220E-02	–1.1145E-02 ± 0.31%	0.2072%	0.67
	5	–1.02465E-02	–1.0243E-02 ± 0.16%	–0.0341%	–0.21
	6	–5.52936E-03	–5.5350E-03 ± 0.16%	0.1021%	0.64
	7	–5.74877E-04	–5.7564E-04 ± 0.29%	0.1327%	0.46
	8	–3.41791E-05	–3.3591E-05 ± 1.14%	–1.7205%	–1.54
Pu-240	1	2.76277E-06	2.7656E-06 ± 1.50%	0.1026%	0.07
	2	2.68133E-05	2.6776E-05 ± 0.44%	–0.1390%	–0.32
	3	6.58184E-04	6.5929E-04 ± 0.19%	0.1681%	0.88
	4	–2.78063E-04	–2.7880E-04 ± 0.48%	0.2652%	0.55
	5	–2.56448E-04	–2.5651E-04 ± 0.29%	0.0241%	0.08
	6	–1.38045E-04	–1.3822E-04 ± 0.29%	0.1267%	0.44
	7	–1.43624E-05	–1.4478E-05 ± 0.62%	0.8050%	1.29
	8	–8.57349E-07	–8.3399E-07 ± 2.39%	–2.7246%	–1.17

SENSMG results for a three-group, one-isotope test problem proposed by Kiedrowski and Brown[6] are given in Appendix B.

VI. Summary and Future Work

This report came about from the observation that MCNP's KSEN (a Monte Carlo code) and SENSMG/PARTISN (a deterministic code) computed very different sensitivities of k_∞ to the same input isotopic fission χ vectors. The values of k_∞ were also different, but not nearly as different as the sensitivities. This report shows that the differences are due to the way each code uses the isotopic fission χ vectors.

None of the differences arise if the test material has only one isotope or if PARTISN uses a fission χ matrix. The differences may also be masked if different nuclear data are used in the comparison, such as "continuous energy" vs. multigroup. Some combination of these probably explains why previous comparisons of Monte Carlo and deterministic sensitivities to χ did not seem to find this effect. Another explanation is that studies may have looked at covariances rather than sensitivities, as in Ref. 16, where there were many sources of overall differences.

Monte Carlo simulations of the analytic problems of Ref. 13 will fail if multi-isotope versions are constructed. How badly they fail will depend on the specific isotopic cross sections chosen.

This report proposes a new `fissdata` option for PARTISN that would allow it to replicate multigroup MCNP results for verification.

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References

1. Ivan A. Kodeli and Slavko Slavič, "SUSD3D Computer Code as Part of the XSUN-2017 Windows Interface Environment for Deterministic Radiation Transport and Cross-Section Sensitivity-Uncertainty Analysis," *Science and Technology of Nuclear Installations*, **2017**, 16 pages (2017); https://doi.org/10.1155/2017/1264736.

2. Toshihiro Yamamoto, "Eigenvalue Sensitivity Analysis Capabilities with the Differential Operator Method in the Superhistory Monte Carlo Method," *Annals of Nuclear Energy*, **112**, 150–157 (2018); https://doi.org/10.1016/j.anucene.2017.10.002.

3. Toshihiro Yamamoto and Hiroki Sakamoto, "A Monte Carlo Technique for Sensitivity Analysis of Alpha-Eigenvalue with the Differential Operator Sampling Method," *Annals of Nuclear Energy*, **127**, 178–187 (2019); https://doi.org/10.1016/j.anucene.2018.12.012.

4. W. Haeck, D. K. Parsons, M. C. White, T. G. Saller, and J. A. Favorite, "Comparison of Monte Carlo and Deterministic Solvers for k_{eff} and Sensitivity Calculations," *Proceedings of the International Conference on the Physics of Reactors* (PHYSOR'18), CD-ROM, Cancun, Mexico, April 22–26 (2018).

5. W. Haeck, D. K. Parsons, M. C. White, T. G. Saller, and J. A. Favorite, "A Comparison of Monte Carlo and Deterministic Solvers for k_{eff} and Sensitivity Calculations," Los Alamos National Laboratory report LA–UR–17-31177 (December 1, 2017); http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-17-31177.

6. Brian C. Kiedrowski and Forrest B. Brown, "Adjoint-Based k-Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo," *Nuclear Science and Engineering*, **174**, *3*, 227–244 (2013); https://doi.org/10.13182/NSE12-46.

7. Brian C. Kiedrowski, "Analytic, Infinite-Medium Solutions for Point Reactor Kinetics Parameters and Reactivity Perturbations," Los Alamos National Laboratory Report LA–UR–10–01803 (2010); https://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-10-01803.

8. Jeffrey A. Favorite, "SENSMG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff}, and α Using PARTISN," *Nuclear Science and Engineering*, **192**, *1*, 80–114 (2018); https://doi.org/10.1080/00295639.2018.1471296.

9. Jeffrey A. Favorite, "(U) SENSMG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff}, and α Using PARTISN," XCP-3:17–009(U), Los Alamos National Laboratory report LA–UR–16–28943, Rev. 4 (March 1, 2018).

10. R. E. Alcouffe, R. S. Baker, J. A. Dahl, E. J. Davis, T. G. Saller, S. A. Turner, R. C. Ward, and R. J. Zerr, "PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System," Los Alamos National Laboratory report LA–UR–17–29704 (Revised March 2018).

11. C. J. Werner, ed., "MCNP User's Manual, Code Version 6.2," Los Alamos National Laboratory report LA–UR–17–29981 (October 17, 2017).

12. Christopher J Werner, ed., "MCNP® User's Manual, Code Version 6.2," Los Alamos National Laboratory report LA–UR–17-29981, Rev. 0 (Oct. 27, 2017).

13. Avneet Sood, R. Arthur Forster, and D. Kent Parsons, "Analytical Benchmark Test Set for Criticality Code Verification," *Progress in Nuclear Energy*, **42**, *1*, 55–106 (2003); https://doi.org/10.1016/S0149-1970(02)00098-7.

14. Jeffrey A. Favorite, Zoltán Perkó, Brian C. Kiedrowski, and Christopher M. Perfetti, "Adjoint-Based Sensitivity and Uncertainty Analysis for Density and Composition: A User's Guide," *Nuclear Science and Engineering*, **185**, *3*, 384–405 (2017); https://doi.org/10.1080/00295639.2016.1272990.

15. Forrest B. Brown, "New Tools to Prepare ACE Cross-section Files for MCNP Analytic Test Problems," Los Alamos National Laboratory report LA–UR–16–24290 (2016); https://laws.lanl.gov/vhosts/mcnp.lanl.gov/pdf_files/la-ur-16-24290.pdf.

16. Ivan Kodeli, Andrej Trkov, Roberto Capote, Yasunobu Nagaya, and Vladimir Maslov, "Evaluation and Use of the Prompt Fission Neutron Spectrum and Spectra Covariance Matrices in Criticality and Shielding," *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **610**, *2*, 540–552 (2009); https://doi.org/10.1016/j.nima.2009.08.076.

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APPENDIX A
INPUT FILES FOR THE EIGHT-GROUP PROBLEM

SENSMG INPUT FILE

The SENSMG source code was modified to run this problem using reflective boundary conditions on the left and right and a mesh spacing of 0.0005 cm.

```
two-isotope slab
slab keff
mendf71x
1 / no of materials
1 94239 -0.96 94240 -0.04  /
-14.00 / densities
 1 / no of shells
 0.  1.  /
 1          / material nos
 0          / number of edit points
 0          / number of reaction-rate ratios
```

The following command line was used to run the input file above:

```
${SENSMG} -i slab -fissdata 2 -srcacc_no for+adj -epsi 1.e-10 -isn 256
-isct 0 -ngroup 8 -np 1 -chinorm full
```

PARTISN INPUT FILE

```
     2     0     0     0     0
two-isotope slab
 forward input file, keff
/ * * * * block i * * * *
 igeom=slab isn= 256 ngroup=    8
 niso=     1 mt=     1 nzone=     1
 im=     1 it=  2000
 t
/ * * * * block ii * * * *
 xmesh=  0.00000000E+00
         1.00000000E+00
 xints=
  2000
 zones=
         1
 t
/ * * * * block iii * * * *
 lib=odninp
 iht=   3 ihs=  11 ihm=  18
 ifido=-1 ititl=1
 maxord= 0
 names= i01
 lng=  8
 t
 siga              nusigf            sigt         mat,ord=  1  0
```

```
 7.49873771887E-02 4.20262201025E-01 2.07447078103E-01 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 1.05433631486E-01 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 6.96711039442E-02 3.76765004145E-01
 2.05056209030E-01 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 1.07009233990E-01 6.42365037265E-03 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 6.52405920965E-02 2.23275161975E-01 2.69044540668E-01 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 1.60490772626E-01 9.33714816219E-03
 6.32052883103E-03 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 6.32103251116E-02 1.88404664872E-01
 2.57480199333E-01 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 1.75915963912E-01 2.92154180331E-02 1.40949930964E-02 1.06738809190E-02
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 5.78891927806E-02 1.52790264322E-01 3.44195793408E-01 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 2.78020458178E-01 1.39082292958E-02
 1.07238177895E-02 3.80915138827E-03 2.74792372725E-03 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 6.41361484524E-02 1.51867709797E-01
 4.47249273556E-01 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 3.79264936909E-01 8.19042840113E-03 4.25274941249E-03 3.21066841230E-03
 1.07887432574E-03 8.17310595375E-04 0.00000000000E+00 0.00000000000E+00
 1.15281472405E-01 1.98199435823E-01 5.75704886855E-01 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 4.57161694187E-01 3.84280700113E-03
 9.29222237681E-05 1.80802616423E-04 1.52350847177E-04 5.08912445270E-05
 3.88346179857E-05 0.00000000000E+00 5.28069517660E-01 8.34089233119E-01
 1.03762844403E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
 5.09558926372E-01 3.26172026397E-03 5.38119296023E-06 2.79182517040E-06
 1.21289854518E-05 1.09208632690E-05 4.81287882857E-06 3.94036479149E-06
/ * * * * block iv * * * *
 matspec=atdens
 matls= m01   i01  1.;
 assign= zone01   m01  1.;
 zonetemp= 2.5301E-08 ;
 t
/ * * * * block v * * * *
 ievt=1 isct=0
 ibl=1 ibr=1 / reflective
 epsi= 1.00E-10 balp=1
 norm=1.0
 npeg=2
 rmflux=1 raflux=1
 iitm=999
 iitl=0 oitm=9999
 srcacc=no
 nofxup=1
```

```
 ith=0 xsectp=2
 chi=
  1.49363021298E-04 1.78070263975E-03 3.69685780267E-01 5.10006815990E-01
  8.96953917406E-02 2.71948263655E-02 1.41155054718E-03 7.55694295334E-05 ;
 t
/ * * * * block vi * * * * *
 ajed=0
 zned=1 igrped=0
 rsfnam=
  "flux" ;
 rsfe=
    8r 1. ;
 t
```

SCRIPT TO COMPUTE ISOTOPIC MULTIGROUP CROSS SECTIONS FOR MCNP

```
#!/bin/csh
module purge
module use /usr/projects/mcnp/modules
module load mcnp6/6.2
rm -rf mg01u mg02u
# unperturbed, pu239
simple_ace_mg.pl -zaid 99901.01m -file mg01u \
  -comment "Pu239, mendf71x, 8 groups, unpert" \
  -groups 8 \
  -f 2.40930845102E+00 2.28823681097E+00 1.86473550810E+00 1.77325651832E+00
1.53649079087E+00 1.54471813788E+00 2.01889327615E+00 8.55454601826E+00 \
  -nu 4.95668948182E+00 4.67905866546E+00 3.40969075323E+00
3.04597604775E+00 2.92430883736E+00 2.89714089923E+00 2.89453717683E+00
2.87747580459E+00 \
  -t 5.88197652690E+00 5.81368478658E+00 7.63012347214E+00 7.30285764937E+00
9.76643792247E+00 1.26932608645E+01 1.63773342859E+01 2.96673421849E+01 \
  -c 2.26121459162E-03 2.37106946395E-03 3.14178704076E-03 3.58364381989E-02
1.58926450926E-01 3.25557806684E-01 1.34079883025E+00 6.82591257150E+00 \
  -s  3.00271605878E+00 1.81819704507E-01 1.68870990053E-01 2.86162137397E-
01 7.40195071989E-02 2.22650805374E-02 1.07553379797E-03 1.12836307964E-04
0.00000000000E+00 3.04857083342E+00 2.55073756180E-01 3.83439823580E-01
1.02676957832E-01 2.93106793967E-02 1.40797827604E-03 1.37388208365E-04
0.00000000000E+00 0.00000000000E+00 4.56009222024E+00 8.18473523810E-01
3.00318763232E-01 9.02390088495E-02 4.31194070269E-03 3.12874042132E-04
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 4.97569585415E+00
3.92635117116E-01 1.19930419689E-01 5.15156530170E-03 3.51692709372E-04
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
7.83780694579E+00 2.30386863223E-01 2.74447627589E-03 8.24572991601E-05
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
0.00000000000E+00 1.07131424244E+01 1.09727960522E-01 1.15029470324E-04
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
0.00000000000E+00 0.00000000000E+00 1.29230419460E+01 9.46006951528E-02
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 1.42868829726E+01 \
  -chi 1.49276717160E-04 1.78016124404E-03 3.69685272745E-01 5.10009192676E-
01 8.96941317783E-02 2.71948534090E-02 1.41154433842E-03 7.55670925349E-05 \
```

```
  -e 1.700000E+01 1.350000E+01 1.000000E+01 2.232000E+00 5.000000E-01
1.840000E-01 2.480000E-02 3.350000E-03 1.670000E-04
# unperturbed, pu240
simple_ace_mg.pl -zaid 99902.01m -file mg02u \
  -comment "Pu240, mendf71x, 8 groups, unpert" \
  -groups 8 \
  -f 2.29423676702E+00 2.17875573727E+00 1.68768121811E+00 1.30433602860E+00
1.62257936804E-01 8.48466840518E-02 8.42876685085E-02 1.63367029871E-01 \
  -nu 4.94155007398E+00 4.65805941769E+00 3.37505947114E+00
3.01743735615E+00 2.90292740532E+00 2.89830998188E+00 2.89732495391E+00
2.89717068490E+00 \
  -t 5.90585618284E+00 5.84985918738E+00 7.62078382066E+00 7.27635482734E+00
9.62850342005E+00 1.24458630020E+01 1.50947846349E+01 2.36041451597E+01 \
  -c 9.72423762252E-04 1.39146003667E-03 2.35262996820E-02 8.98237562636E-02
1.83869974942E-01 4.93801874377E-01 1.00481150035E+00 5.04890338423E+00 \
  -s 2.68253008040E+00 1.90520079432E-01 4.29187445605E-01 7.01204092975E-01
1.72112903892E-01 4.51763491064E-02 1.72225442484E-03 8.54085591845E-05
0.00000000000E+00 2.69894823034E+00 4.98939650392E-01 7.91970239538E-01
2.36854369382E-01 6.15595191523E-02 2.29229289767E-03 1.14766132779E-04
0.00000000000E+00 0.00000000000E+00 4.33961496875E+00 1.07042114426E+00
3.95567530067E-01 1.10604326067E-01 4.52605137315E-03 2.33239022888E-04
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 5.30327978031E+00
4.37416518189E-01 1.36797817267E-01 4.54314010165E-03 1.57651813109E-04
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
9.00472486383E+00 2.77650630647E-01 3.95201623549E-07 7.29409724816E-09
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
0.00000000000E+00 1.17752794563E+01 9.08779776306E-02 1.05816097811E-03
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
0.00000000000E+00 0.00000000000E+00 1.39638600823E+01 4.18249318607E-02
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 0.00000000000E+00
0.00000000000E+00 0.00000000000E+00 0.00000000000E+00 1.83918759178E+01 \
  -chi 1.62431462900E-04 1.86268246581E-03 3.69762630789E-01 5.09646930779E-
01 8.98861791534E-02 2.71907313481E-02 1.41249069636E-03 7.59233051220E-05 \
  -e 1.700000E+01 1.350000E+01 1.000000E+01 2.232000E+00 5.000000E-01
1.840000E-01 2.480000E-02 3.350000E-03 1.670000E-04
```

MCNP INPUT FILE

```
kinfinity, 8 groups, 2 isotopes
1   1   0.03526255669   1 -2     imp:n=1
99  0                  (-1:2)    imp:n=0

*1 px 0.
*2 px 1.

mode n
rand gen=2 seed=1000000001
mgopt f 8
prdmp j 500
kcode 6400000 2.9 100 1100
sdef x=d1
si1  0. 1.
sp1  0. 1.
```

```
xs1   99901.01m 1e+06        mg01u      0 1 1 123  0 0 2.5301e-08
xs2   99902.01m 1e+06        mg02u      0 1 1 123  0 0 2.5301e-08
m1    99901.01m 0.03385770516
      99902.01m 0.00140485153
kopts   blocksize = 5
ksen01   xs   cell=1 rxn= -4 constrain=no
         erg=1.6700E-04 3.3500E-03 2.4800E-02 1.8400E-01
             5.0000E-01 2.2320E+00 1.0000E+01 1.3500E+01 1.7000E+01
ksen02   xs   cell=1 rxn= -4 constrain=yes
         erg=1.6700E-04 3.3500E-03 2.4800E-02 1.8400E-01
             5.0000E-01 2.2320E+00 1.0000E+01 1.3500E+01 1.7000E+01
print -30
```

SPECTRUM WEIGHTING FUNCTIONS

Group	Pu-239	Pu-240
1	7.764844070E-02	7.765239730E-02
2	3.315532630E-02	3.315586090E-02
3	8.680570310E-01	8.680599750E-01
4	3.195349230E+00	3.195348650E+00
5	1.315065040E+00	1.315065250E+00
6	2.314158420E+00	2.314144660E+00
7	2.311274120E+00	2.311267420E+00
8	3.461271880E+00	3.461267720E+00

APPENDIX B
SENSMG RESULTS FOR A THREE-GROUP TEST PROBLEM

Kiedrowski and Brown presented a three-group, one-isotope k_∞ test problem for which they compared MCNP KSEN sensitivities of k_∞ to χ with analytic values as a verification of the then-new KSEN feature.[6] The three-group cross sections were fictitious.

SENSMG is not set up to accept fictitious cross sections easily, but it can be done. The procedure is as follows:

1. Run a SENSMG input having the desired geometry and number of isotopes.
2. Convert the forward PARTISN input deck by entering the fictitious material macroscopic cross sections in "`lib=odninp`" format and using an atom density of 1 for each material in block 4. Set `niso` in block 1 to the number of materials. Set the material χ vector using `chivec` in block 3 or `chi` in block 5 (the latter is required for this problem because $\nu\sigma_f^g$ is zero for some groups).
3. Run the forward PARTISN input deck in directory `for` with output file name `for_out`.
4. Convert the adjoint PARTISN input deck by using an atom density of 1 for each material in block 4. Set `niso` in block 1 to the number of materials. Set the material χ vector as in step 2.
5. Run the adjoint PARTISN input deck in directory `adj` with output file name `adj_out`.
6. Convert the "cross section" PARTISN input deck by entering the fictitious material macroscopic cross sections in "`lib=odninp`" format and using an atom density of 1 for each material in block 4. Use the first eight characters of each entry in the `names` array in block 3.
7. Run the "cross section" PARTISN input deck in directory `xs1` with output file name `xs1_out`.
8. Run the SENSMG input from step 1 with "`-use_existing yes`" on the command line.

For this problem, the forward and adjoint inputs also included "`ibl=1 ibr=1`", reflecting boundary conditions, in block 5.

Due to PARTISN's eight-character limit on the length of entries in the `names` array in block 3, the SENSMG source code has to be modified to implement this procedure. In source file `rdsnxedt.F`, uncomment the two lines between "`DEBUG_ALEX`" and comment the line above.

The source code was also modified to run with a mesh spacing of 0.0005 cm, as in Sec. V. An angular quadrature of S_{256} and a convergence criterion of 10^{-8} were used.

The nuclear data used in this test problem are given in Table B.I. The density is 1 atom/b·cm. The analytic value for k_∞ is unity [Eq. (2)]. The SENSMG/PARTISN value is also unity (to seven digits).

Table B.I. Nuclear Data for the Three-Group Test Problem.[6]

g	σ_t^g	σ_c^g	$\nu\sigma_f^g$	χ^g	$\sigma_s^{g\to1}$	$\sigma_s^{g\to2}$	$\sigma_s^{g\to3}$
1	2	1/2	0	5/8	1	1/2	0
2	4	1	0	1/4	0	1	2
3	4	1/2	4	1/8	0	0	2

The unconstrained SENSMG sensitivities are compared with analytic sensitivities in Table B.II. Constrained SENSMG sensitivities (using full normalization) are compared with analytic sensitivities in Table B.III. In both tables, the SENSMG results are exact to the number of decimals printed in the output.

Table B.II. Unconstrained Sensitivities of k_∞ to χ, Deterministic (No Normalization) (%/%).

Group	Analytic[6]	SENSMG	Difference
1	+5/12	4.166667E-01	0.000008%
2	+1/3	3.333333E-01	–0.000010%
3	+1/4	2.500000E-01	0.000000%

Table B.III. Constrained Sensitivities of k_∞ to χ, Deterministic (Full Normalization) (%/%).

Group	Analytic[6]	SENSMG	Difference
1	–5/24	–2.083333E-01	–0.000016%
2	+1/12	8.333333E-02	–0.000004%
3	+1/8	1.250000E-01	0.000000%

The Monte Carlo results published in Ref. 6 also agree with the analytic values, demonstrating that, as shown in this report, when there is only one isotope in the material, Eqs. (1) and (10) have the same solution and sensitivities.